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# HYDROGEN FLOW MODEL IN POROUS MEDIA FOR UNDERGROUND HYDROGEN STORAGE (UHS)

**Erik TENGBLAD[1], Laura ASENSIO[2], Vicente NAVARRO[3]**

## ABSTRACT

The increasing need for renewable energy storage due to the fluctuating nature of sources like wind and solar power requires efficient large-scale energy storage solutions. Underground Hydrogen Storage (UHS) in porous media, such as depleted gas fields and saline aquifers, presents a promising method for storing hydrogen, which has a high energy content per unit mass (Gessel, 2023).

Numerical modelling is crucial for the proper study and design of UHS. It allows for the prediction of the behaviour of stored hydrogen within the reservoir, as well as its interaction with cushion gas or formation water. This predictive capability is essential for optimizing injection and extraction processes, minimizing losses, and improving storage efficiency (Sainz-Garcia et al., 2017). A comprehensive model is proposed to simulate hydrogen transport in porous media, incorporating factors such as gas solubility, density, and the effects of temperature, pressure, and salinity.

Therefore, a Thermo-Hydro-Chemical-Mechanical (THCM) tool with a triple porosity model (Navarro et al., 2024, 2020), that enhances the characterization of the behaviour of such storage systems, with special consideration of hydro-mechanical effects has been implemented. The aim of this work is to present this tool along with its qualification by simulating reservoir-scale tests, which include hydrogen injection into a depleted gas reservoir.

**Keywords:** underground hydrogen storage, numerical modelling, hydro-mechanical couplings, triple porosity.

## INTRODUCTION

The use of hydrogen as an energy carrier is largely conditioned by the ability to efficiently store significant amounts of hydrogen, with underground reservoirs being the most promising strategy (Gessel, 2023; Zivar et al., 2021).

In the absence of reservoir-scale tests or operational projects for Underground Hydrogen Storage (UHS), information from natural gas storage is valuable (Gessel, 2023). However, this information must be treated with caution because of the important differences between the physico-chemical properties of methane and hydrogen. This makes numerical simulation of UHS systems (UHSS) crucial for investigating their performance and feasibility.

Recent advances in numerical simulation of UHSS behaviour have been made by Sainz-Garcia et al. (2017), Hagemann et al. (2016), and Cai et al. (2022), among others. These studies have been fundamental in analysing the feasibility of UHSS and developing new numerical models.

Flexibility and efficiency of simulation codes are essential due to the uncertainty in the characterisation of UHSS properties, which requires scaling the complexity of the model to the available information. Multi-physics models provide this adaptability by allowing different physics to be mobilised without changing the source code, allowing researchers to focus on developing conceptual models rather than numerical tools.

## NUMERICAL TOOL

Looking for a flexible and open interface development environment that allows the implementation of various differential equations and constitutive models (Navarro et al., 2019), Comsol Multiphysics (2023) was chosen for the development of the 'X2H' code. This software uses symbolic algebra for automatic differentiation and allows a very simple and intuitive programming language, since the formulas are written directly in a natural way, thus achieving a double objective: improving the computational performance and simplifying the tasks, making the codes clearer and more robust.

The aim of this work is to present a numerical tool, "X2H", which improves the characterization of the UHSS behaviour, along with its qualification by reproducing the simulation of hydrogen injection in a depleted gas reservoir by Hagemann et al. (2016).

1 Geoenvironmental Group, Universidad de Castilla-La Mancha, Ciudad Real, Spain. Erik.Tengblad@uclm.es
2 Dr., Geoenvironmental Group, Universidad de Castilla-La Mancha, Ciudad Real, Spain. Laura.Asensio@uclm.es
3 Prof., Geoenvironmental Group, Universidad de Castilla-La Mancha, Ciudad Real, Spain. Vicente.Navarro@uclm.es

## CONCEPTUAL MODEL

### Transport Model

For simplicity, the study considers a non-deformable medium with isothermal conditions, where the gas phase consists of hydrogen, methane, and water vapor.

The liquid phase is modelled as a generic saline solution containing dissolved hydrogen and methane. These simplifications aim to balance model accuracy with computational efficiency, facilitating comparisons with other codes and focusing on the core aspects of UHSS transport behaviour.

Hydrodynamic dispersion of hydrogen, methane, and vapor in the gas phase is approximated using molecular diffusion, following Fick's law, and is calculated as a function of porosity, tortuosity, and the diffusion coefficient in the gas. The gas saturation degree is treated as a state function related to the liquid saturation degree. A monotonic drying process is considered, using van Genuchten's retention law (1980). The intrinsic permeabilities of the gas and liquid phases are assumed to be equal. The salinity of the liquid is considered negligible, allowing the use of pure water properties for density and dynamic viscosity. The specific discharge of the gas and liquid phases is calculated using Darcy's law.

### State Variables and Balance Equations

To determine state variables, mass balance equations for hydrogen, methane, and water are solved, assuming no source or sink terms. The total mass flow is calculated for each component, with the gas and liquid densities derived from state variables and concentrations.

To mitigate mass conservation problems that may arise when simulating frontal propagation in the UHSS, CM uses advanced finite element techniques, where the domain is divided into smaller finite elements, allowing complex problems to be handled by solving differential equations within each of these elements.

CM allows the use of text files (libraries) to define the constitutive relationships and state functions of each of the hydrogen, methane and water balances solved, while defining the mass balance equations by specifying the conservative flux, source term and mass coefficient.

Material properties, geometry and other parameters, together with initial and boundary conditions, are defined from libraries, and the implicit boundary conditions are defined by coupled ordinary differential equations, allowing flexible and efficient implementation of the model.

## QUALIFICATION

For validation of the X2H numerical model, and in the absence of experimental data for the UHSS, the results of other validated models with similar dimensions as a full-scale test are used as a reference for better assessing the capabilities of X2H.

### Hydrogen injection into a depleted reservoir

This case reproduces the simulation of hydrogen injection in a depleted gas reservoir carried out by Hagemann et al. (2016). The domain represents a small anticlinal structure with idealized conditions, assuming a homogeneous and isotropic porous medium.

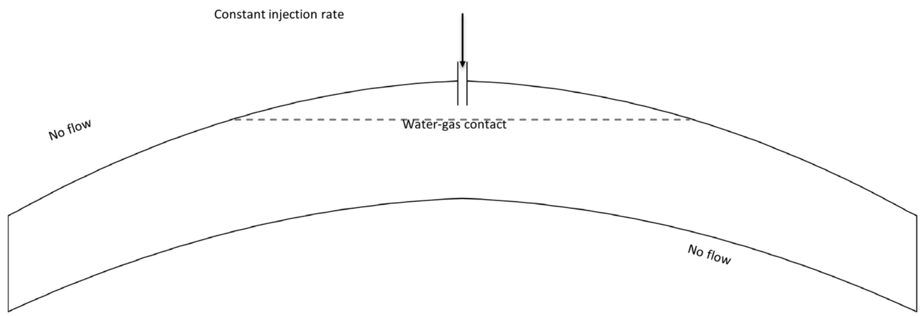



**Figure 1** *Geometry, initial conditions and boundary conditions (adapted from Hagemann et al. (2016), Fig. 3)*

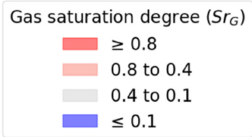
## NUMERICAL IMPLEMENTATION

Comsol Multiphysics (CM) was chosen as the implementation platform because of its symbolic algebra capabilities and ease of programming; in addition, CM allows derivatives to be calculated in an automated manner using symbolic differentiation.

Hydrogen is injected at the top centre of the reservoir, with impermeable top and bottom boundaries and constant water pressure at the external boundaries. The initial gas pressure is 6 MPa, with a water-gas contact at 22 meters from the top centre. A porosity of 0.2, a tortuosity of

1 and an intrinsic permeability of $9.87 \cdot 10^{-14}$ m$^2$, are assumed.

The van Genuchten model (1980) is used to characterize soil retention properties, with an air entry pressure of 0.1 MPa and a residual liquid saturation of 0.2. The parameter $n_{VG}$ was estimated to be 3.03 by fitting the initial gas saturation values to those of Hagemann et al. (2016).



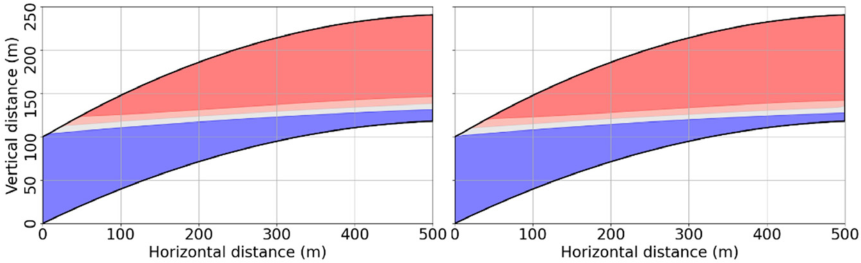




**Figure 2** *Legend, also for Figure 3-5; Case 1: 0.1 mol·s$^{-1}$ / $2.7 \cdot 10^9$s (≈ 85.5 years). Hagemann et al. (2016) Fig 4 (b) vs X2H*

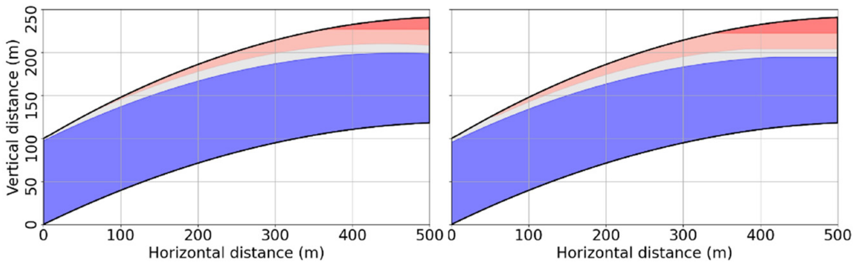



**Figure 3** *Case 2: 2 mol·s$^{-1}$ / $2.6 \cdot 10^7$s (≈ 9 months). Hagemann et al. (2016) Fig 4 (c) vs X2H*

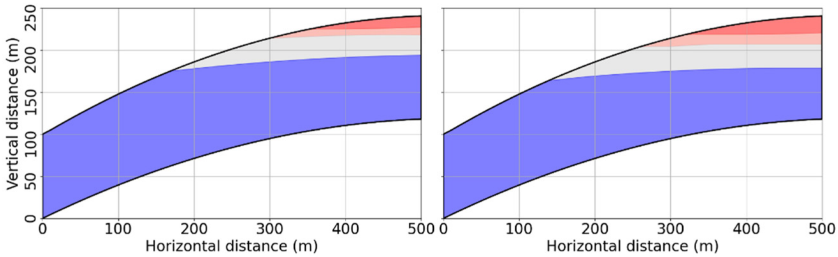



**Figure 4** *Case 3: 100 mol·s$^{-1}$ / $1.25 \cdot 10^6$s (≈ 14.5 days). Hagemann et al. (2016) Fig 4 (d) vs X2H*

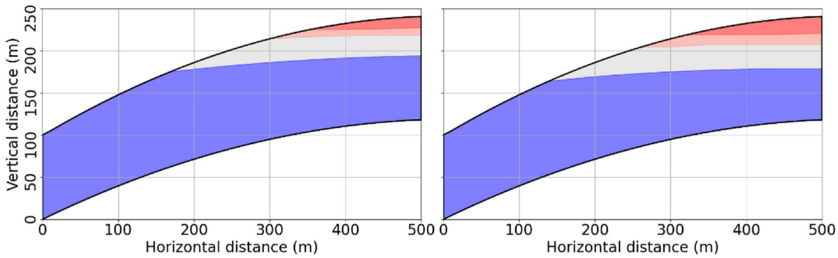



**Figure 5** *Case 4: 100 mol·s$^{-1}$ / $3.2 \cdot 10^6$s (≈ 37 days). Hagemann et al. (2016) Fig 4 (e) vs X2H*

To test the ability of X2H to simulate several conditions, different hydrogen injection rates and simulation times were reproduced.

The results of the gas saturation degree ($Sr_G$) obtained with X2H, are given as the right graph in each of Figures 2 to 5, were compared with those of Hagemann et al. (2016), shown as left graph at each Figure.

The comparison showed demonstrates an excellent fit, as illustrated in Figs. 2 to 5. This indicates that the X2H tool accurately reproduces the conditions and results of the original simulation by Hagemann et al. (2016), which validates its effectiveness in modelling hydrogen injection scenarios in UHSS.

## CONCLUSIONS

The X2H model demonstrates exceptional capabilities in simulating the behaviour of Underground Hydrogen Storage Systems (UHSS). The numerical environment provided by Comsol Multiphysics (2023) provides a flexible and reliable platform for implementing complex differential equations and constitutive models. The use of symbolic algebra for automatic differentiation improves computational performance and simplifies programming tasks. The qualification example of hydrogen injection into a depleted reservoir shows that X2H can accurately predict gas saturation levels and capture the dynamics of hydrogen transport in porous media. The model's ability to handle different injection rates and times and compare favourably with established models like those of Hagemann et al. (2016) underscores its reliability and effectiveness.

Overall, X2H stands out as a powerful tool for researchers and engineers, offering a comprehensive and efficient solution for studying and optimizing UHSS. Its flexibility, accuracy, and ease of use make it an invaluable asset in the field.

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